Convection 3D

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1 Equations

1.1 Mass conservation

$$\frac{\partial c_i}{\partial t} = -\vec{\nabla}.\vec{N}_i + R_i \tag{1}$$

with

$$\vec{N}_i = c_i\vec{v} - \sum_j D_{ij}\vec{\nabla}c_j - w_i c_i \vec{\nabla}U \tag{2}$$

1.2 Poisson's equation

$$\vec{\nabla}^2 U + \frac{F}{\epsilon}\sum_i z_i c_i = 0 \tag{3}$$

1.3 Butler-Volmer kinetics

$$v = k_{ox}\exp\left[\frac{\alpha_{ox}nF}{RT}(V-U)\right]c_{red} - k_{red}\exp\left[-\frac{\alpha_{red}nF}{RT}(V-U)\right]c_{ox} \tag{4}$$

2 Element matrix

2.1 Convection

2.1.1 Fluctuation in node

$$\Delta c_i^m = \sum_e \alpha_e^m \Phi_e$$

2.1.2 Element contribution to fluctuation in node

$$\begin{aligned}
\Phi &= \int_V -\vec{v}.\vec{\nabla}c_i dV \\
&= -\left(\frac{\vec{n}^1 c_i^1 + \vec{n}^2 c_i^2 + \vec{n}^3 c_i^3 + \vec{n}^4 c_i^4}{3}\right).\vec{v}_{av} \\
&= -\left(k^1 c_i^1 + k^2 c_i^2 + k^3 c_i^3 + k^4 c_i^4\right)
\end{aligned}$$

- One target (e.g. node 1)

$$\alpha^1 = 1$$

$$\alpha^2 = \alpha^3 = \alpha^4 = 0$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = - \left[\begin{array}{cccc} k^1 & k^2 & k^3 & k^4 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \\ c_i^4 \end{array} \right\} \tag{5}$$

- Two target: LDA-scheme (e.g. nodes 1 and 2)

$$\alpha^1 = \frac{k^1}{k^1 + k^2}$$

$$\alpha^2 = \frac{k^2}{k^1 + k^2}$$

$$\alpha^3 = \alpha^4 = 0$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = - \left[\begin{array}{cccc} \frac{\left(k^1\right)^2}{k^1+k^2} & \frac{k^1 k^2}{k^1+k^2} & \frac{k^1 k^3}{k^1+k^2} & \frac{k^1 k^4}{k^1+k^2} \\ \frac{k^2 k^1}{k^1+k^2} & \frac{\left(k^2\right)^2}{k^1+k^2} & \frac{k^2 k^3}{k^1+k^2} & \frac{k^2 k^4}{k^1+k^2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \\ c_i^4 \end{array} \right\} \tag{6}$$

- Two target: N-scheme (e.g. nodes 1 and 2)

Note: the distribution coefficients are undefined!

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = - \left[\begin{array}{cccc} k^1 & 0 & \frac{k^1 k^3}{k^1+k^2} & \frac{k^1 k^4}{k^1+k^2} \\ 0 & k^2 & \frac{k^2 k^3}{k^1+k^2} & \frac{k^2 k^4}{k^1+k^2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \\ c_i^4 \end{array} \right\} \tag{7}$$

- Three target: LDA-scheme (e.g. nodes 1, 2 and 3)

$$\alpha^1 = -\frac{k^1}{k^4}$$

$$\alpha^2 = -\frac{k^2}{k^4}$$

$$\alpha^3 = -\frac{k^3}{k^4}$$

$$\alpha^4 = 0$$

$$\left\{\begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array}\right\} = \left[\begin{array}{cccc} \frac{\left(k^1\right)^2}{k^4} & \frac{k^1 k^2}{k^4} & \frac{k^1 k^3}{k^4} & k^1 \\ \frac{k^2 k^1}{k^4} & \frac{\left(k^2\right)^2}{k^4} & \frac{k^2 k^3}{k^4} & k^2 \\ \frac{k^3 k^1}{k^4} & \frac{k^3 k^2}{k^4} & \frac{\left(k^3\right)^2}{k^4} & k^3 \\ 0 & 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \\ c_i^4 \end{array}\right\} \tag{8}$$

- Three target: N-scheme (e.g. nodes 1, 2 and 3)

Note: the distribution coefficients are undefined!

$$\left\{\begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array}\right\} = \left[\begin{array}{cccc} -k^1 & 0 & 0 & k^1 \\ 0 & -k^2 & 0 & k^2 \\ 0 & 0 & -k^3 & k^3 \\ 0 & 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \\ c_i^4 \end{array}\right\} \tag{9}$$

2.1.3 Examples: binary electrolyte

- One target (node 1)

$$\left\{\begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \\ \Delta c_A^4 \\ \Delta c_B^4 \\ \Delta U^4 \end{array}\right\} = \left[\begin{array}{cccccccccccc} -k^1 & 0 & 0 & -k^2 & 0 & 0 & -k^3 & 0 & 0 & -k^4 & 0 & 0 \\ 0 & -k^1 & 0 & 0 & -k^2 & 0 & 0 & -k^3 & 0 & 0 & -k^4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \\ c_A^4 \\ c_B^4 \\ U^4 \end{array}\right\} \tag{10}$$

- Two target: N-scheme (nodes 1 and 2)

$$
\left\{\begin{array}{c}\Delta c_A^1\\ \Delta c_B^1\\ \Delta U^1\\ \Delta c_A^2\\ \Delta c_B^2\\ \Delta U^2\\ \Delta c_A^3\\ \Delta c_B^3\\ \Delta U^3\\ \Delta c_A^4\\ \Delta c_B^4\\ \Delta U^4\end{array}\right\} = \begin{bmatrix}
-k^1 & 0 & 0 & 0 & 0 & 0 & \frac{k^1k^3}{k^1+k^2} & 0 & 0 & \frac{k^1k^4}{k^1+k^2} & 0 & 0\\
0 & -k^1 & 0 & 0 & 0 & 0 & 0 & \frac{k^1k^3}{k^1+k^2} & 0 & 0 & \frac{k^1k^4}{k^1+k^2} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & -k^2 & 0 & 0 & \frac{k^2k^3}{k^1+k^2} & 0 & 0 & \frac{k^2k^4}{k^1+k^2} & 0 & 0\\
0 & 0 & 0 & 0 & -k^2 & 0 & 0 & \frac{k^2k^3}{k^1+k^2} & 0 & 0 & \frac{k^2k^4}{k^1+k^2} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}\left\{\begin{array}{c}c_A^1\\ c_B^1\\ U^1\\ c_A^2\\ c_B^2\\ U^2\\ c_A^3\\ c_B^3\\ U^3\\ c_A^4\\ c_B^4\\ U^4\end{array}\right\} \tag{11}
$$

- Three target: N-scheme (nodes 1, 2 and 3)

$$
\left\{\begin{array}{c}\Delta c_A^1\\ \Delta c_B^1\\ \Delta U^1\\ \Delta c_A^2\\ \Delta c_B^2\\ \Delta U^2\\ \Delta c_A^3\\ \Delta c_B^3\\ \Delta U^3\\ \Delta c_A^4\\ \Delta c_B^4\\ \Delta U^4\end{array}\right\} = \begin{bmatrix}
-k^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & k^1 & 0 & 0\\
0 & -k^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & k^1 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & -k^2 & 0 & 0 & 0 & 0 & 0 & k^2 & 0 & 0\\
0 & 0 & 0 & 0 & -k^2 & 0 & 0 & 0 & 0 & 0 & k^2 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & -k^3 & 0 & 0 & k^3 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -k^3 & 0 & 0 & k^3 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}\left\{\begin{array}{c}c_A^1\\ c_B^1\\ U^1\\ c_A^2\\ c_B^2\\ U^2\\ c_A^3\\ c_B^3\\ U^3\\ c_A^4\\ c_B^4\\ U^4\end{array}\right\} \tag{12}
$$

3 Element jacobian

3.1 Convection

Zero contribution.